

Classical simulation of short time many-body dynamics

Alvaro M. Alhambra

(Instituto de Fisica Teorica CSIC -Madrid)



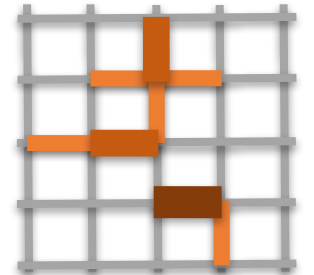
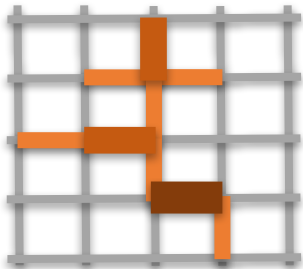
w/ Dominik Wild

(Max Planck Institute for Quantum Optics)



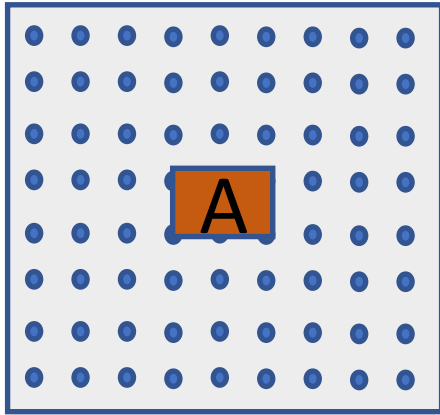
(arXiv:2210:11490)

Accepted in PRX Quantum



Simulating many-body dynamics

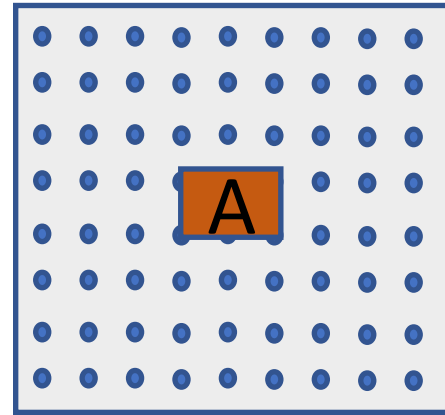
$$U = e^{-itH} \quad H = \sum_i h_i$$



$$A(t) = e^{-iHt} A e^{iHt}$$

Simulating many-body dynamics

- Time evolution operator: $U = e^{-itH}$ $H = \sum_i h_i$
- Observable: $A(t) = e^{-iHt} A e^{iHt}$
- Initial state: $|\Phi\rangle = \bigotimes_i |\phi_i\rangle$
- Goal:



$$|\langle \Phi | A(t) | \Phi \rangle - f(t)| \leq \epsilon$$

Computational problem

- Local Hamiltonian on N particles + few-body observable

$$|\langle \Phi | A(t) | \Phi \rangle - f(t)| \leq \epsilon$$

Classically easy (P)

$$t = \mathcal{O}(1)$$

...

Classically hard +
quantum easy (BQP)

$$t = \text{poly}(N)$$

...

Quantum hard

$$t \stackrel{??}{=} \exp(N)$$

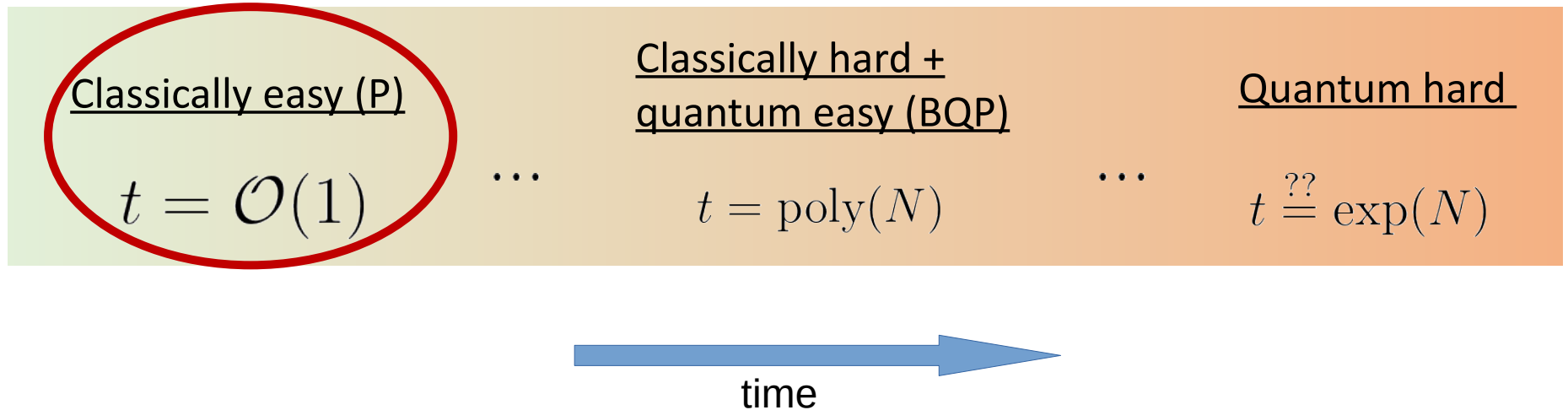


time

Computational problem

- Local Hamiltonian on N particles + few-body observable

$$|\langle \Phi | A(t) | \Phi \rangle - f(t)| \leq \epsilon$$



How do we study this problem classically?

- Exact diagonalization (small systems)
- Tensor networks (short times, one dimension)

- Many other methods....(model-specific?)

$$A(t) = e^{-iHt} A e^{iHt}$$

-

- This talk: cluster expansion ← short times, but very accurate and analytically tractable

Quantum dynamics: simple or not?



A HUGE matrix
you cannot
diagonalize

$$U \in (\mathbb{C}^d)^{\otimes N}$$



The exponential of
a “simple” local
operator

$$U = e^{-itH}$$

$$H = \sum_i h_i$$



Taylor expansion and classical computation

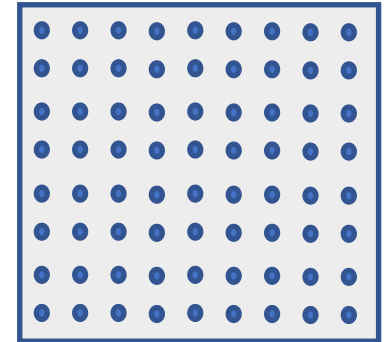
$$|F(t) - F_m(t)| \leq e^{-\mathcal{O}(m)}$$

$$F(t) = \sum_{m=0}^{\infty} \frac{K_m}{m!} t^m$$

$$F(t)_M = \sum_{m=0}^M \frac{K_m}{m!} t^m$$

Ingredients:

- Prove convergence of Taylor series for high enough degree (analyticity).
- Estimate cost of calculating Taylor coefficients.
- Computed Taylor series gives approximation.



Cluster expansion: main idea

- Taylor series expansions for quantities defined on lattices.

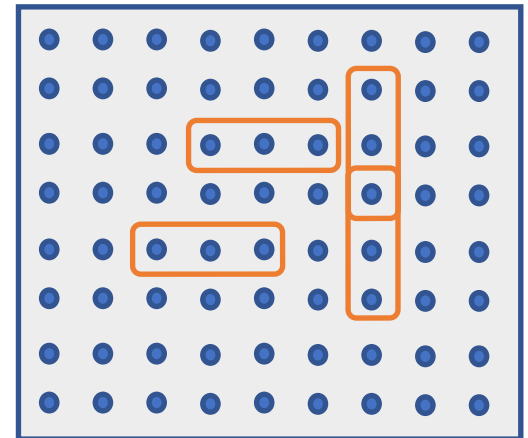
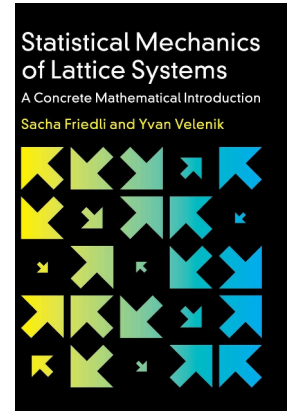
$$\log Z \equiv \log \text{Tr}[e^{-\beta H}] = \sum_m \frac{K_m^{(\beta)}}{m!} \beta^m \quad e^{-\beta H} = \mathbb{I} - \beta H + \frac{\beta^2}{2} H^2 + \dots$$

- Find efficient way of writing & computing the Taylor moments in terms of *clusters*

$$H = \sum_X h_X \quad K_m^{(\beta)} = \sum_{\mathbf{w}} \prod(\dots) \text{Tr}[h_1 \dots h_n]$$
$$\|h_X\| \leq 1$$

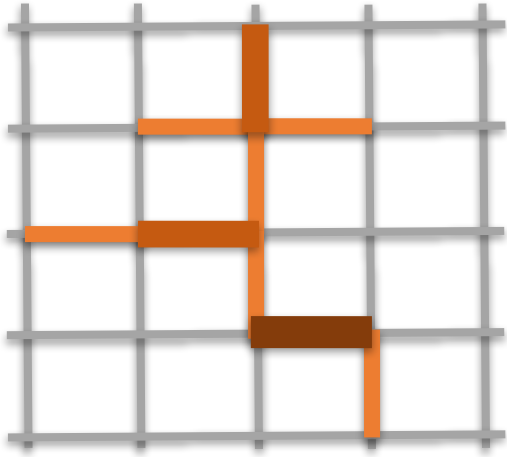
- **CLUSTER**: A multiset of Hamiltonian terms

$$\mathbf{W} = \{h_1, h_1, h_2, \dots, h_l, h_l\}$$



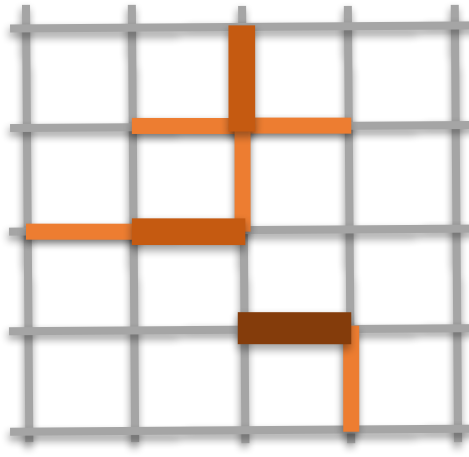
Types of clusters

- Connected



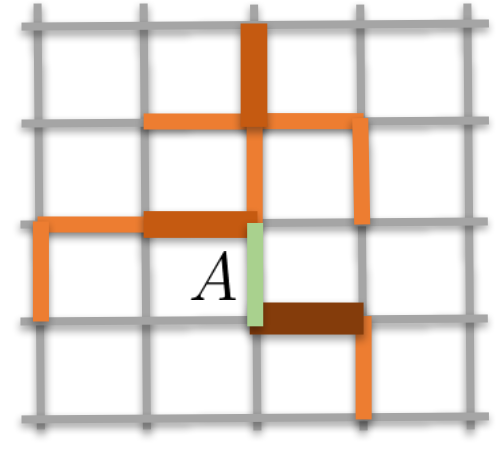
$$\mathbf{W} \in \mathcal{G}_m$$

- Disconnected



$$\mathbf{W} \in \mathcal{C}_m \setminus \mathcal{G}_m$$

- Connected to A



$$\mathbf{W} \in \mathcal{G}_m^A$$

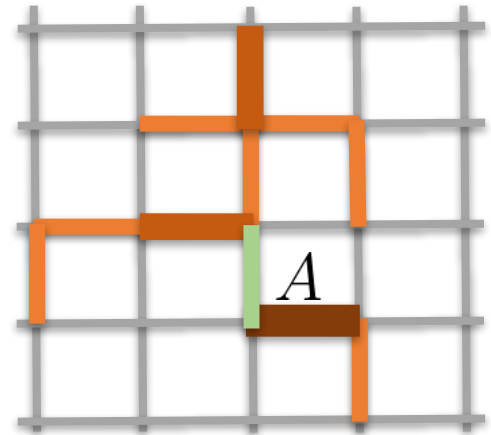
$$\mathbf{W} = \{h_1, h_1, h_2, \dots, h_l, h_l\}$$

Heisenberg time evolution

- Classical simulation of

$$\begin{aligned} \langle \Phi | e^{-itH} A e^{itH} | \Phi \rangle &= \sum_{m=0}^{\infty} \frac{(it)^m}{m!} \langle \Phi | [H, [H, \dots [H, A]] | \Phi \rangle \\ &= \sum_{m=0}^{\infty} \frac{(it)^m}{m!} \sum_{\mathcal{G}_m^A} \langle \Phi | [h_{X_1}, [h_{X_2}, \dots [h_{X_m}, A]] | \Phi \rangle \end{aligned}$$
$$H = \sum_i h_i$$

- Taylor expansion in terms of *connected* clusters



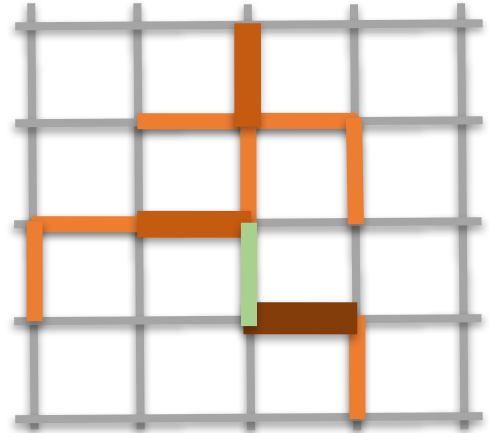
Heisenberg time evolution

- Classical simulation of

$$\begin{aligned} \langle \Phi | e^{-itH} A e^{itH} | \Phi \rangle &= \sum_{m=0}^{\infty} \frac{(it)^m}{m!} \langle \Phi | [H, [H, \dots [H, A]] | \Phi \rangle \\ &= \sum_{m=0}^{\infty} \frac{(it)^m}{m!} \sum_{\mathcal{G}_m^A} \langle \Phi | [h_{X_1}, [h_{X_2}, \dots [h_{X_m}, A]] | \Phi \rangle \end{aligned}$$

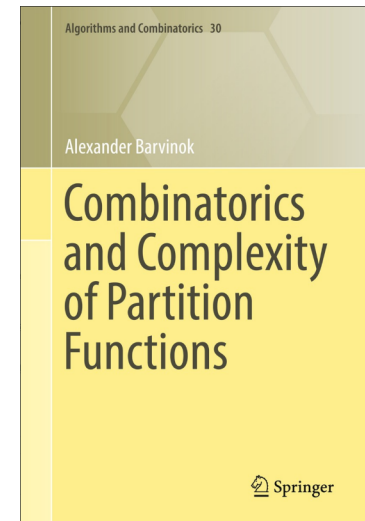
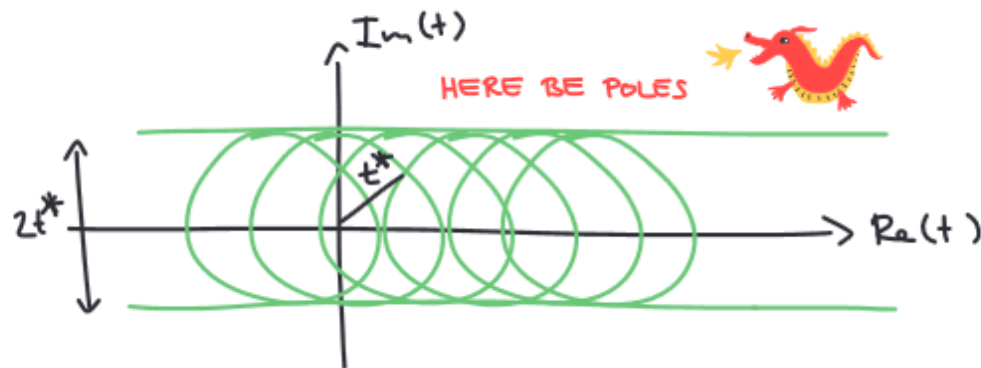
- Count connected clusters: $|\mathcal{G}_A^m| \leq e^{\mathcal{O}(m)}$
- Weight of each cluster: $m! 2^m \|A\|$
- Taylor series (and algorithm) for short times

$$t \leq t^* \quad \left| \langle \Phi | A(t) | \Phi \rangle - \sum_{m=0}^M \frac{t^m}{m!} K_m \right| \leq \frac{(t/t^*)^M}{1 - (t/t^*)} \|A\|$$



Arbitrary times: analytic continuation

- Function is analytic on a strip, not just a disk. $|\langle e^{-itH} A e^{itH} \rangle| \leq \|A\|$
- Analytic continuation (Barvinok '16, Harrow et al. 1910.09071).
- We can use Taylor series at the origin to calculate any later point, with **overhead**.
- Idea: use series of a function that maps disk to rectangle.



Arbitrary times: main result

- Series converges, but much more slowly (exponentially badly in time)
- RESULT: for arbitrary times, there is a classical algorithm that outputs $f(t)$

$$|\langle \Phi | e^{-itH} A e^{itH} | \Phi \rangle - f(t)| \leq \epsilon$$

- With runtime

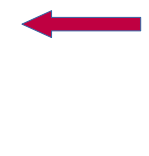
$$\left(\exp(\mathcal{O}(t)) \frac{1}{\epsilon} \right)^{\exp(\mathcal{O}(t))} \leftarrow$$

Arbitrary times: main result

- Series converges, but much more slowly (exponentially badly in time)
- RESULT: for arbitrary times, there is a classical algorithm that outputs $f(t)$

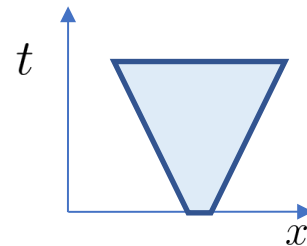
$$|\langle \Phi | e^{-itH} A e^{itH} | \Phi \rangle - f(t)| \leq \epsilon$$

- With runtime

$$\left(\exp(\mathcal{O}(t)) \frac{1}{\epsilon} \right)^{\exp(\mathcal{O}(t))}$$


- Remark: for $t = \mathcal{O}(1)$, runtime is $\text{poly}(\epsilon^{-1})$
- Previously: Lieb-Robinson lightcone method has runtime

$$e^{\mathcal{O}(l^D)} \sim e^{\mathcal{O}((vt + \log(1/\epsilon))^D)}$$



Fidelity / Loschmidt echo

$$\log \langle \Phi | e^{-itH} | \Phi \rangle \text{ vs. } \log [\text{Tr} e^{-\beta H}]$$

- KEY INSIGHT: with product states also only connected clusters contribute

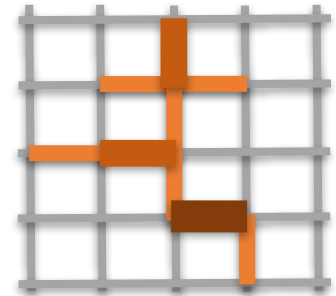
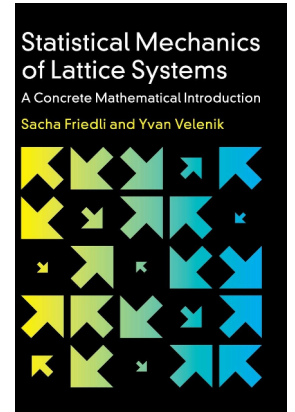
$$|\Phi\rangle = |\phi\rangle^{\otimes N}$$

- Result: classical algorithm for Loschmidt echo

$$|\log \langle \Phi | e^{iHt} | \Phi \rangle - \sum_{m=0}^M \frac{t^m}{m!} K_m| \leq \epsilon \quad t \leq t^*$$

$$M = \mathcal{O}(\log(N/\epsilon))$$

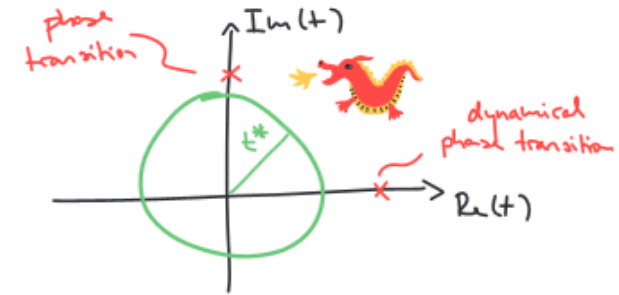
$$\text{runtime} = \text{poly}(N/\epsilon)$$



Some physical consequences:

- Result: analyticity and efficient algorithm for

$$\log \langle \Phi | e^{-itH} | \Phi \rangle \quad t \leq t^*$$



- So it takes at least t^* to become orthogonal to initial state
- Strengthening over previous Quantum Speed Limits (Mandelstam-Tamm, Margolus-Levitin)

$$t_{QSL} \geq t^* = \mathcal{O}(1) \quad \text{vs.} \quad t_{QSL} \geq \mathcal{O}(1/\sqrt{N})$$

- Dynamical phase transitions (Heyl 1709.07461): t^* is a lower bound to how fast they occur. (in analogy with thermal phase transitions)
- **BONUS**: concentration bounds (Chernoff) for short-time evolved states.

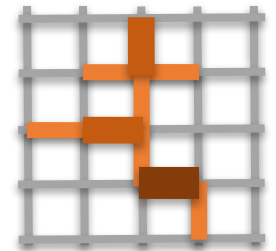
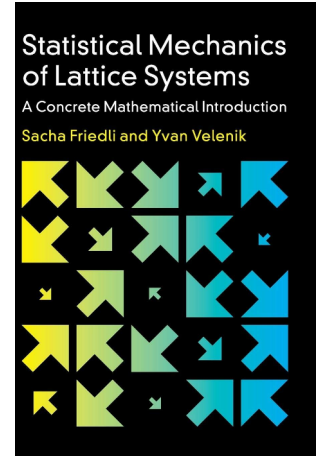
Computational complexity of quantum dynamics

Evolution time	$\leq t^*$	$\mathcal{O}(1)$	$\mathcal{O}(\text{polylog}(N))$	$\mathcal{O}(\text{poly}(N))$
$\langle A(t) \rangle$	P	P	??	BQP-complete
$\log \langle e^{-itH} \rangle$	P	#P-hard	#P-hard	#P-hard
$\langle e^{-itH} \rangle$	P	??	??	BQP-complete

- Complexity of simulating to small additive error $\epsilon = 1/\text{poly}(N)$
- #P hard -> Galanis et al 2005.01076
- BQP hardness: standard arguments + de las Cuevas (1104.2517)

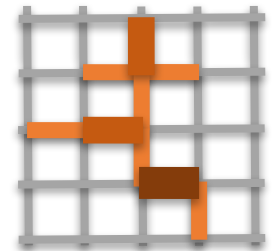
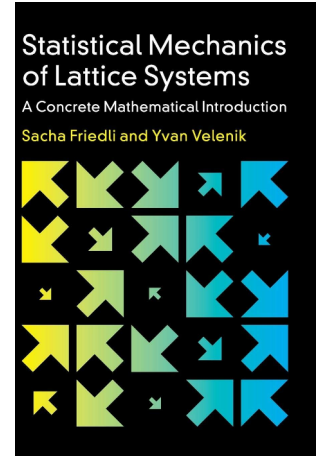
Conclusions

- Cluster expansion: versatile and well-studied tool for partition functions + related problems.
 - Shows convergence of Taylor approximation and yields efficient algorithms.
 - Works for many different interaction graphs.
- Here: it also works for problems of **quantum dynamics**.
- Versatile technique for classical simulation of many quantum problems.



Conclusions

- Cluster expansion: versatile and well-studied tool for partition functions + related problems.
 - Shows convergence of Taylor approximation and yields efficient algorithms.
 - Works for many different interaction graphs.
- Here: it also works for problems of **quantum dynamics**.
- Versatile technique for classical simulation of many quantum problems.



arXiv:2210.11490

Thanks!!